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D.L. McDowell and R.W. Neu

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School of Materials Science and Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0405

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14. ABSTRACT
Damage and plastic deformation accumulation in fretting fatigue occurs within a depth of a few crystallographic grains. Therefore, more accurate assumptions concerning length scale, damage volume, and the material model are needed to establish a more solid physical foundation necessary for next generation fretting fatigue damage prediction. Major thrusts include: (1) development and implementation of a 3-D crystal viscoplasticity model for Ti-6Al-4V, (2) realistic 3-D fretting simulations that capture influence of key microstructure features, including distinct phase properties and crystallographic texture, and (3) experimental characterization of fretting experiments to both validate fretting simulation results and identify additional features to incorporate in the crystal viscoplasticity model and fretting simulations.

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MICROSTRUCTURE AND 3-D EFFECTS IN FRETTING FATIGUE OF TI ALLOYS AND NI-BASE SUPERALLOYS

FA9550-04-1-0418

Faculty: D.L. McDowell and R.W. Neu
Graduate Students: M. Zhang, X. Huang, J.R. Mayeur
The George W. Woodruff School of Mechanical Engineering
School of Materials Science and Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0405

Abstract

Damage and plastic deformation accumulation in fretting fatigue occurs within a depth of a few crystallographic grains. Therefore, more accurate assumptions concerning length scale, damage volume, and the material model are needed to establish a more solid physical foundation necessary for next generation fretting fatigue damage prediction. Major thrusts include: (1) development and implementation of a 3-D crystal viscoplasticity model for Ti-6Al-4V, (2) realistic 3-D fretting simulations that capture influence of key microstructure features, including distinct phase properties and crystallographic texture, and (3) experimental characterization of fretting experiments to both validate fretting simulation results and identify additional features to incorporate in the crystal viscoplasticity model and fretting simulations.

Development of a Crystal Viscoplasticity Model for Ti-6Al-4V

Improvements and extensions to our crystal viscoplasticity model for Ti-6Al-4V continue to be made each year. This year, a major extension to 3-D was undertaken. Our initial two-dimensional crystal plasticity model of duplex Ti-6Al-4V employed a planar triple slip idealization (Goh et al., 2006a and references therein). This was a pioneering effort to show effect of grain orientation distribution, grain size and geometry, as well as the phase distribution and their arrangement in fretting contact problems, suggesting that the role of micro-textures (and indeed primary α size and orientation) might be significant in resisting fretting fatigue (Goh et al., 2006b).

The 2-D crystal plasticity model was extended to a full 3-D version by Mayeur and McDowell (2006) as reported in last year's annual report. The 3-D model is capable of representing arbitrary crystallographic textures, the unique crystallography of the constituent phases, anisotropy of slip system strengths, and non-planar dislocation core structures. These features are essential to capturing the deformation behavior of these materials due to the low symmetry of the hcp crystal structure and the resulting anisotropic properties. These material models are coded in FORTRAN as ABAQUS User MATerial subroutines. Consideration of more realistic microstructure morphologies using Voronoi tessellation coupled with simulated annealing techniques have also been considered (Zhang et al., 2006a; 2006b; 2006c).

It is well known that fatigue crack formation within Ti-6Al-4V is associated with the impingement of slip on boundaries and decohesion of shear bands. To account for these mechanisms, our 3-D crystal viscoplasticity model will be further enhanced to address the shear localization and the slip bands. The new crystal plasticity model will use a two-potential flow rule and take the dislocation density as the internal variable to determine the hardening and softening behavior of Ti-6Al-4V. Several new features such as shear band spacing, evolution of nanoporosity in the shear bands will be considered. The local enriched finite element method will be used to model the shear bands in primary α phase. Then fatigue performance metrics based on deformation response within the heterogeneous microstructure will be more physically based.

Fretting Simulations

Fretting contacts, presently considering the partial slip regime, are simulated by a finite element model of a rigid cylinder on an elastic-crystal viscoplastic half-space. The half-space is modeled as duplex Ti-6Al-4V, a polycrystalline alloy consisting of equiaxed primary α grains and secondary lamellar α+β grains. Both 2-D finite element simulations using a generalized plane strain assumption, which is limited to line contact problems, and more recently fully 3-D finite element simulations have been conducted. Both employ the fully 3-D crystal viscoplasticity model.

2-D finite element simulations

Various realistic 3-D crystallographic textures have been considered and reported in last year's report. The deformation fields generated by fretting are quantified in terms of cumulative effective plastic strain distributions and plastic strain maps (Mayeur et al., 2005a; 2005b; 2006a; 2006b). The 2-D simulations are carried out for several microstructural realizations with emphasis placed on understanding how texture and tangential load affect the fatigue life.

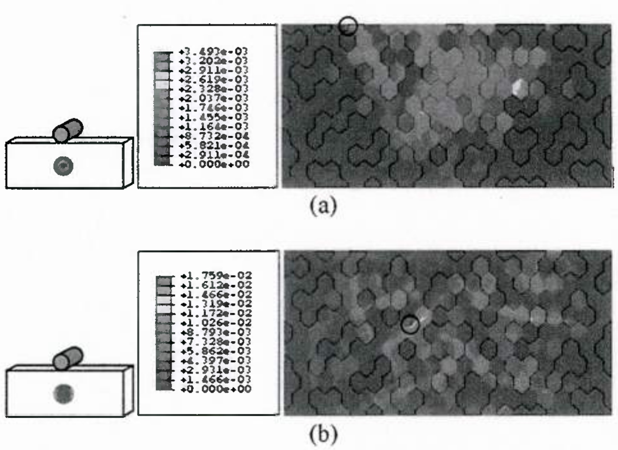


Figure 1. Cumulative effective plastic strain distributions at the end of 3rd cycle, (a) basal texture and (b) transverse texture.

Illustrative results are displayed for the basal and transverse textured materials in Fig. 1 (Mayeur et al., 2006a). The locations of maximum cumulative effective plastic strain have been highlighted in Fig. 1. For all three types of textures considered, plastic ratcheting is observed to be the dominant mode of cyclic plastic deformation. This is in agreement with previous results from crystal plasticity fretting simulations with idealized 2-D textures (Goh et al., 2006a and references therein). The basal textured material exhibits the least amount of plastic ratcheting and correspondingly the most homogeneous distribution of cumulative effective plastic strain. This is direct result of all of the grains for this type of texture being favorably aligned for soft modes of deformation. As a by-product of the relatively homogeneous nature of deformation in the basal textured material, it is able to reach a state of elastic shakedown much earlier than mixed-types of textures. The transverse and basal/transverse textured materials exhibit significantly different behavior. Both of these materials display a highly heterogeneous distribution of cumulative effective plastic strain in the subsurface region (see Figure 2(b)). The plastic strain is partitioned in vein-like "soft" regions of the microstructure in which relatively few favorably oriented grains are surrounded by unfavorably oriented primary α grains and/or the lamellar α+β grains. The confined nature of the plastic strain for the transverse and basal/transverse textured materials leads to continued cyclic plastic ratcheting as smaller regions of the material are required to accommodate the plastic deformation. The cumulative effective plastic strain is considerably greater in these regions. The results clearly demonstrate the importance of the various sources of microstructural heterogeneity in the surface layers. The main sources of microstructural heterogeneity include the distribution of phases, slip system strength anisotropy, and crystallographic texture.

Several fatigue indicator parameters have been considered (Mayeur et al., 2006b). Plastic strain-based critical plane parameters are the most relevant. In addition, both single point and volume-averaged calculations have been considered. The latter tend to temper strong gradients in the near surface stress-strain field and illuminate size effects in fatigue crack formation. The appropriate size of the averaging volume also depends on the microstructure (grain size, phase distribution, contiguity, etc.), the contact loading conditions, and even the coefficient of friction. The parameters are related to the cycles to crack formation according to a modified Coffin-Manson law using data generated in the Air Force High Cycle Fatigue program.

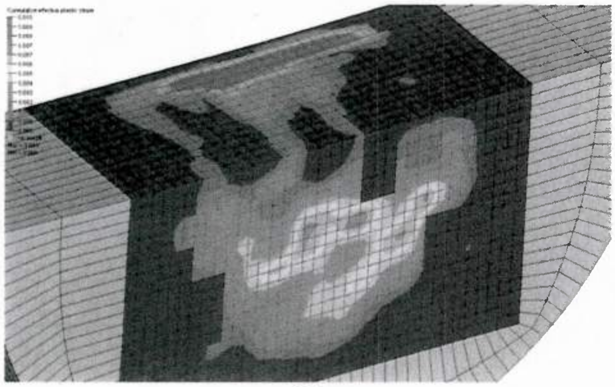
3-D finite element simulations

Fully 3-D FE simulations are conducted to investigate the applicability of the generalized plane strain assumption for line contact problems and to allow for more complex fretting configurations such as capturing the experimentally observed edge effects along the contact.

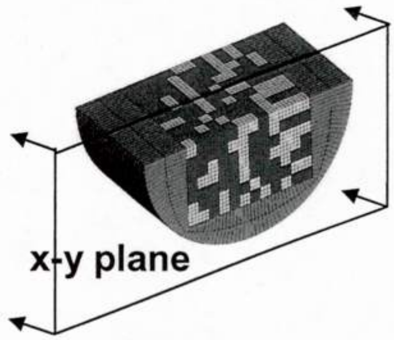
Four textures, basal, transverse, basal/transverse and random textures, were considered in this study to examine the effects of the texture on the fretting fatigue behavior of Ti-6Al-4V (Zhang et al., 2006). The contours show localization of the cumulative plastic strain. One case is shown in Fig. 2. Some grains significantly yield while the neighboring grains still undergo elastic deformation. The significant contact edge effect can be observed near the surface because in this case the contacting body is shorter in the z-direction than the substrate. At the x-y plane of the half space, the peak cumulative plastic strain is located in the subsurface region, in agreement with the results obtained from the 2-D simulations for a comparable loading case when the tangential force is relatively low.

Plastic ratcheting is observed to be the dominant mode of cyclic plastic deformation, which is in consistent with the previous results, as summarized in Table 1 for various texture realizations under the same fretting loading. N_p denotes the number of elements that plastically deform. It is concluded that the transverse and basal/transverse textures have higher resistance to fretting fatigue since there are fewer number of plastically deformed elements and lower values of maximum cumulative plastic strain.

In the coming year, additional simulations will be conducted to further quantify the effects of loading and microstructure parameters on the fretting fatigue life. The applicability of the generalized plane strain assumption for line contact problems will be examined via 3-D simulations. To correlate the simulation results with experimental data, realistic finite element meshes will be built directly from EBSD measurements, obtained from fretting experiments.



(a)



(b)

Figure 2. (a) Distribution of cumulative effective plastic strain after three transverse loading cycles for basal texture for the case: normal load $P/P_y = 1$ and tangential force amplitude is $Q/P_y = 0.1$, where P_y is the normal force for initial yielding using von Mises criterion. (b) Illustration of the section view showing the two-phase microstructure. The x-y plane passes through the center of the model.

Table 1. Summary of plastic strain behavior of the entire crystal plasticity region.

Texture	N_p	Elastic shakedown (% of elements)	Cyclic plasticity (% of elements)	Combined cyclic and ratcheting (% of elements)	Ratcheting (% of elements)
Basal	15979	13.9	0.01	9.24	76.9
Transverse	11762	24.4	0.02	2.81	72.8
Basal/ Transverse	11231	25.7	0.01	1.54	72.8
Random	14223	15.9	0	7.96	76.1

Experimental Characterization of Fretting Damage

The high temperature fretting machine (DURIP grant F49620-03-1-0260), shown in Fig. 3, continued to be used in the past year to better understand the role of microstructure in the fretting damage process. As mentioned in the last year's report, this new machine has a considerably higher normal force capacity (4500 N) than typical tribometers used in conventional fretting studies, which results in a larger volume of microstructure being distressed by the fretting process facilitating microstructure characterization using pressures relevant to the dovetail attachment.

In the past year, a baseline study of fretting of Ti-6Al-4V on Ti-6Al-4V in point and line contact at room temperature in air was conducted spanning the partial slip, mixed fretting, and gross slip regimes of fretting. Cracks are typically observed in the mixed fretting regime. The mouth of the cracks are typically wide, indicative of the large plastic ratchet strains in the surface layer. These results are consistent with fretting simulations indicating that the greatest plastic strain accumulation is near the interfaces between the different grains.

Two methods were used to establish the running condition response of Ti-6Al-4V on Ti-6Al-4V: a conventional multiple specimen approach and an incremental displacement method using a single specimen (Huang and Neu, 2006). It was found that the displacement amplitude corresponding to the transition from partial to gross slip is the same for both methods, and the normal load, at least for values of P/P_y ranging from 1.5 to 3.9, does not significantly affect the coefficient of friction. The running condition and material response at 260°C is essentially the same as the room temperature response (Huang and Neu, 2006). In our heavy loaded cases, multiple cracks are observed near the edges of contact at 10^4 cycles under mixed fretting conditions. A significant oxide debris layer forms by 10^6 cycles, which is not present at 10^4 cycles. The depth of the oxide debris layer is comparable to the depth of cracks formed at 10^4 cycles, suggesting that crack formation and filling of cracks with oxide debris precedes generation of complete oxide debris layers.

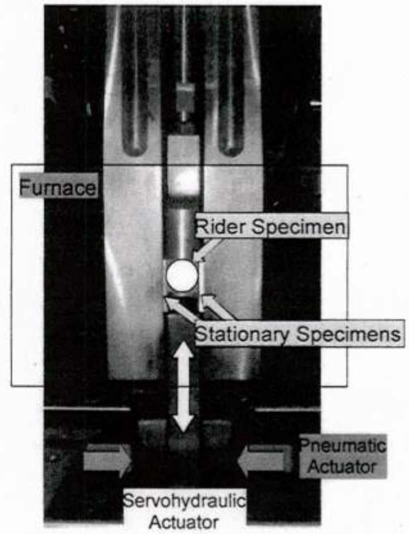


Figure 3. Fretting test machine.

Automated electron backscatter diffraction (EBSD) is used to establish how fretting spatially evolves microtexture and the relationship between crystallographic orientation, grain boundaries and formation of subgrains and cracks in the fretting process volume (Swalla and Neu, 2006). It is a useful tool to quantify evolution of strain-induced microstructural changes due to deformation in the near-surface layers. One notable observation is the appearance of low angle misorientations (<5°) near the fretted surface that tend to increase with increasing slip amplitude (Swalla and Neu, 2006). The development of these intra-grain misorientations in medium to high stacking fault metals is due to the formation of dislocation substructures with accumulated plastic deformation. Presently, different quantifiable measures of these lattice distortions and intra-grain misorientations are being evaluating both on a pure copper as well as on Ti-6Al-4V. The relationship between these intra-grain misorientation parameters and plastic strain appear to be linear. We developed a method to establish the correlation using a shear-dominated torsion experiment, which is more relevant to the shear-dominated loading in fretting and sliding contacts. These methods are being developed to aid in quantitatively interpreting the fretting results and could eventually be used to calibrate material parameters in evolutionary equations in a crystal plasticity model that captures the formation of these dislocation substructure features.

To establish the role of crystallographic orientation on the fretting damage response, a fretting study on single crystal Ni-base superalloy, PWA 1484, was conducted. In particular, fretting was conducted on the (001) crystal plane in two directions representing the extreme responses on this plane: the [100] and [110] crystal directions. A crystallographic effect on the fretting response was observed at highest normal force ($P > P_y$), while there was no crystallographic effect observed at the lower normal force ($P < P_y$). Through EBSD characterization, the orientation dependence in fretting is primarily associated with the orientation dependence of plastic deformation in the near surface material. Hence, crystal plasticity and relevant lower microstructure length scale models are necessary to predict these observations.

It is more appropriate to validate the fretting simulations using results from fretting experiments conducted in inert gas atmosphere since the chemical activity and associated mechanical mixing in the surface layers is not presently addressed in the deformation modeling. To separate the effects of the chemical and mechanical processes, an environmental enclosure is currently under development for conducting experiments in inert or other gaseous environments, from room temperature to 800°C.

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Personnel Supported

Ming Zhang	Graduate Student, Georgia Institute of Technology, Atlanta, GA
Xuan Huang	Graduate Student, Georgia Institute of Technology, Atlanta, GA
Richard W. Neu	Associate Professor, Georgia Institute of Technology, Atlanta, GA
David L. McDowell	Regents' Professor, Georgia Institute of Technology, Atlanta, GA

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